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PATENT NO : 7,199,809 B1

APPLICATION NO.: 09/420,334

ISSUE DATE : April 3, 2007

INVENTOR(S) : Lacy et al.

It is certified that an error appears or errors appear in the above-identified patent and that said Letters Patent is hereby corrected as shown below:

Beginning at Column 29, Line 15 through Column 36, Line 65, Claims 1 through 78 should be replaced with the following 16 claims:

1. A computer-implemented method for generating a library design for a combinatorial library of materials, comprising:

providing a graphical user interface including a workspace for designing a library of materials; defining one or more sources and one or more destinations, each source being electronic data representing a chemical or mixture of chemicals to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

displaying a visual representation of one or more of the one or more defined destinations in the workspace of the graphical user interface, each destination representation including a representation of one or more destination areas, each destination area including one or more cells in the corresponding arrangement;

receiving user input associating each of the one or more sources with one or more of the destination areas;

receiving user input specifying a plurality of equations and associating each of the plurality of equations with one or more of the one or more destination areas;

solving the plurality of equations to calculate one or more amounts of one or more first chemicals or mixtures of chemicals represented by the one or more defined sources to be assigned to one or more cells in the one or more arrangements represented by the one or more defined destinations, the one or more amounts of the one or more first chemicals or mixtures of chemicals to be assigned to a given cell in the one or more arrangements being calculated according to a set of equations comprising a plurality of the equations, the equations in the set of equations being associated with the area or areas that include the cell, the one or more first chemicals or mixtures of chemicals to be assigned to the given cell being determined by the one or more sources associated with the area or areas that include the cell; and

modifying the visual representation of the one or more defined destinations to include a visual indication of the one or more calculated amounts.

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2. The method of claim 1, further comprising:

generating an error indicator signal if the plurality of equations cannot be solved for each cell in the one or more arrangements.

3. The method of claim 1, wherein at least one of the plurality of equations is selected from the group consisting of:

a ratio equation defining an amount of one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of an amount of another chemical or mixture of chemicals to be assigned to the cell;

a volume equation defining an amount of one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of a total volume of a plurality of chemicals or mixtures of chemicals to be assigned to the cell; and

a mass equation defining an amount of one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of a total mass of a plurality of chemicals or mixtures of chemicals to be assigned to the cell.

- 4. The method of claim 1, wherein solving the plurality of equations comprises using matrix algebra techniques to solve the plurality of equations.
 - 5. The method of claim 1, further comprising:

receiving an input defining a gradient mapping, the gradient mapping being electronic data defining a distribution pattern for distributing a second chemical or mixture of chemicals to cells in the one or more arrangements, the distribution pattern including a minimum and a maximum amount of the second chemical or mixture of chemicals to be assigned to any of a plurality of cells of the one or more arrangements and a gradient to be applied between the minimum and maximum amounts of the second chemical or mixture of chemicals across the plurality of cells; and

using the second mapping to calculate amounts of the second chemical or mixture of chemicals to be deposited in each of the plurality of cells;

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wherein modifying the visual representation of the one or more defined destinations comprises modifying the visual representation to include a visual indication of the calculated amounts of the first and second chemicals or mixtures of chemicals.

6. A computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials, the computer program product comprising instructions operable to cause a programmable processor to:

provide a graphical user interface including a workspace for designing a library of materials; define a set of one or more sources and one or more destinations, each source being electronic data representing a chemical or mixture of chemicals to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

display a visual representation of one or more of the one or more defined destinations in the workspace of the graphical user interface, each destination representation including a representation of one or more destination areas, each destination area including one or more cells in the corresponding arrangement;

receive user input associating each of the one or more sources with one or more of the destination areas;

receive user input specifying a plurality of equations and associating each of the plurality of equations with one or more of the destination areas:

solve the plurality of equations to calculate one or more amounts of one or more first chemicals or mixtures of chemicals represented by the one or more defined sources to be assigned to one or more cells in the one or more arrangements represented by the one or more defined destinations, the one or more amounts of the one or more first chemicals or mixtures of chemicals to be assigned to a given cell in the one or more arrangements being calculated according to a set of equations comprising a plurality of the equations, the equations in the set of equations being associated with the area or areas that include the cell, the one or more first chemicals or mixtures of chemicals to be assigned to the given cell being determined by the one or more sources associated with the area or areas that include the cell; and

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modify the visual representation of the one or more defined destinations to include a visual indication of the one or more calculated amounts.

- 7. The computer program product of claim 6, further comprising instructions operable to: generate an error indicator signal if the plurality of equations cannot be solved for each cell in the one or more arrangements.
- 8. The computer program product of claim 6, wherein at least one of the plurality of equations is selected from the group consisting of:
- a ratio equation defining an amount of one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of an amount of another chemical or mixture of chemicals to be assigned to the cell;
- a volume equation defining an amount of one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of a total volume of a plurality of chemicals or mixtures of chemicals to be assigned to the cell; and
- a mass equation defining an amount of one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of a total mass of a plurality of chemicals or mixtures of chemicals to be assigned to the cell.
- 9. The computer program product of claim 6, wherein the instructions operable to cause a programmable processor to solve the plurality of equations comprise instructions to use matrix algebra techniques to solve the plurality of equations.
- 10. The computer program product of claim 6, further comprising instructions operable to: receive an input defining a gradient mapping, the gradient mapping being electronic data defining a distribution pattern for distributing a second chemical or mixture of chemicals to cells in the one or more

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arrangements, the distribution pattern including a minimum and a maximum amount of the second chemical or mixture of chemicals to be assigned to any of a plurality of cells of the one or more arrangements and a gradient to be applied between the minimum and maximum amounts of the second chemical or mixture of chemicals across the plurality of cells; and

use the second mapping to calculate amounts of the second chemical or mixture of chemicals to be deposited in each of the plurality of cells:

wherein the instructions operable to cause a programmable processor to modify the visual representation of the one or more defined destinations include instructions operable to cause a programmable processor to modify the visual representation to include a visual indication of the calculated amounts of the first and second chemicals or mixtures of chemicals.

11. The method of claim 1, further comprising:

receiving user input dividing one or more of the one or more destination representations to define the destination areas.

12. The method of claim 1, further comprising:

in response to the user input specifying and associating the equations, modifying the visual representation of the one or more defined destinations to include a visual indication of the equations associated with the one or more destination areas.

13. The method of claim 1, wherein:

defining the one or more sources comprises associating one or more of the chemicals or mixtures of chemicals with a type representing a class of chemicals to be used in preparing the combinatorial library;

receiving user input specifying a plurality of equations comprises receiving user input specifying one or more of the plurality of equations as a function of the type; and

solving the equations comprises solving the equations specified as a function of the type for a given destination area by substituting the corresponding associated chemical or chemicals associated for the type.

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14. The computer program product of claim 6, further comprising instructions operable to cause a programmable processor to:

receive user input dividing one or more of the destination representations to define the destination areas.

15. The computer program product of claim 6, further comprising instructions operable to cause a programmable processor to:

modify the visual representation of the one or more defined destinations in response to the user input specifying and associating the equations to include a visual indication of the equations associated with the one or more destination areas.

16. The computer program product of claim 6, wherein:

the instructions operable to cause a programmable processor to define the one or more sources comprise instructions operable to cause a programmable processor to associate one or more of the chemicals or mixtures of chemicals with a type representing a class of chemicals to be used in preparing the combinatorial library:

the instructions operable to cause a programmable processor to receive user input specifying a plurality of equations comprise instructions operable to cause a programmable processor to receive user input specifying one or more of the plurality of equations as a function of the type; and

instructions operable to cause a programmable processor to solve the equations comprise instructions operable to cause a programmable processor to solve the equations specified as a function of the type for a given destination area by substituting the corresponding associated chemical or chemicals associated for the type.

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